Experimentally Verified Quantum Device Simulations Based on Multiband Models, Hartree Self-Consistency, and Scattering Assisted Charging

R. Lake, G. Klimeck, R. C. Bowen, C. Fernando, D. Jovanovic, D. Blanks, T. S. Moise, and Y. C. Kao

Corporate R&D, Texas Instruments Incorporated, P.O. Box 655936, MS 134, Dallas, TX 75265
Email: RLAKE@NEMOHP1.CSC.TI.COM *Ph: (214) 995-1176 FAX: (214) 995-2836*

M. Leng and W. R. Frensley

Eric Jonsson School of Electrical Engineering and Computer Science, University of Texas at Dallas, Richardson, TX 75083-0688

Accurate predictions of the I-V characteristics of Esaki diodes, resonant tunneling diodes (RTD), and resonant interband tunneling diodes (RITD) require sophisticated models of bandstructure, charging, and scattering. We present direct comparisons of experimental and simulation data based on single, two, and 10 band models and the world's first calculation of the electrostatic potential obtained *self-consistently with scattering-assisted charging.* This charge results from the incoherent scattering off of alloy disorder, interface roughness, acoustic phonons and polar-optical phonons.

For symmetric RTDs, standard Schrödinger - Poisson models predict 10-40 mV of intrinsic bistability when, in fact, no bistability is experimentally observed. Including exchange-correlation into the Hartree potential eliminates the predicted bistability for some devices [1] but this correction does not work in general. To resolve the inconsistencies between theory and experiment, we developed a model that uses the LDA approximation to include exchange-correlation effects and which accounts for scattering-assisted tunneling in the device current. For low temperature RTDs, the charging of the quantum well in the post-resonance (valley) region of the I-V is determined by incoherent scattering channels. A self-consistent treatment of scattering assisted charging of the well reduces the theoretically calculated width of the bistable region by approximately 50%.

We studied a number of InP lattice matched InGaAs / InAlAs RTDs measured at room temperature. Quantitative agreement between theory and experiment often required an sp3s* model for the bandstructure, a numerical integration over the transverse momentum, and generalized boundary conditions (GBC) [2]. The GBCs were required to model the injection from the emitter states. An sp3s* bandstructure model combined with numerical integration over the transverse momentum was required to simulate the different dispersions in the emitter and well under bias [3]. For these devices, we find that at room temperature, the valley current is determined by thermionic emission through the first excited state in the well. The inclusion of disorder and phonon scattering was unnecessary to match the valley current.

An InAs / AlSb / GaSb RITD was simulated using the two-band k•p model, Hartree self-consistent charging, and the GBCs. The two-band model is sufficient since only the light-hole band of the GaSb couples significantly to the conduction band states in the InAs. But, a calculation of the hole charge combined with self-consistency is required to obtain the post-valley current increase. This current rise results from Zener tunneling of valence band electrons into the conduction band. Our inter-band model does not include scattering or thermalization processes, and this will be required to model the effect of thermionic hole emission on the valley current of these devices [4].

Acknowledgments: We thank Jun Shen at Motorola and John Huber at Yale for the data on the RITD and G. Frazier for incisive editorial comments.

[1] N. Zou et al., *Phys. Rev. B*, **49**, 2193 (1994).
[2] G. Klimeck et al., *Appl. Phys. Lett.*, **67**, 2539 (1995).
[3] T. B. Boykin, Phys. Rev. B, **51**, 4289 (1995).
[4] J. Shen, J. *Appl. Phys.*, **78**, 6220 (1996).

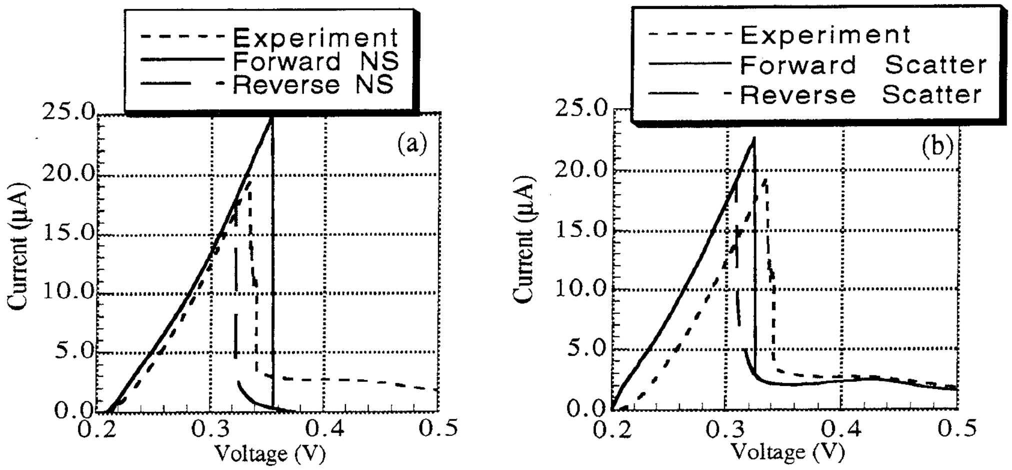

Fig. 1. I-V of a GaAs / AlAs RTD with a 5.66 nm well and 3.1 nm barriers with 20 nm spacer layers separating the barriers from the n+ contacts (T=4.2K). The I-V is calculated self-consistently including the LDA approximation for the exchange-correlation terms without scattering in Fig. (1a) and with scattering in Fig. (1b). Polar optical phonon scattering dominates the valley current. The short dashed line is the experimental data in both figures. Note the shift in the I-V resulting from the real part of the self-energy.

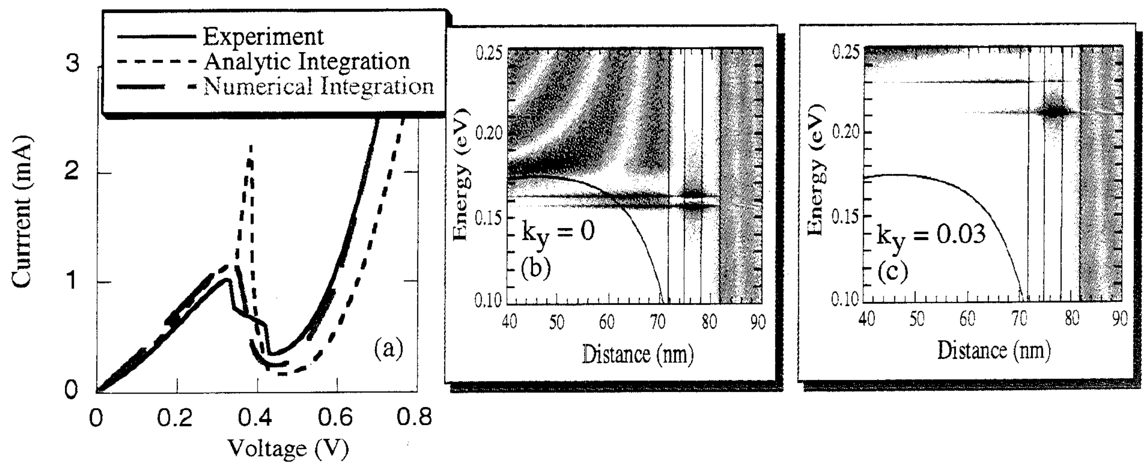

Fig. 2. (a) Experimental and simulated I-Vs of InGaAs / InAlAs RTD. The numerical integration over transverse momentum removes the unphysical peak in the I-V curve and results in quantitative agreement with the entire experimental I-V. (b) For transverse momentum ky = 0, the emitter state and well state align, couple, and split. (c) For transverse momentum ky = 0.03π/a, the emitter and well state do not align.

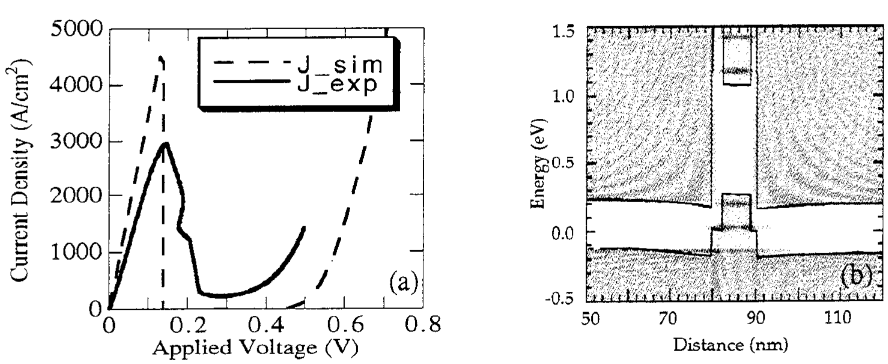

Fig. 3. (a) Experimental and simulated I-V of an InAs/AlSb/GaSb RITD. Hartree self-consistency is required to get the turn-on after the valley current. The turn-on is the result of Zener tunneling of valence electrons into the conduction band (b) Quantization of light-hole states in the well.